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Elementary computer physics, a concentrated one-week course

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A concentrated one-week course (8 hours per day in 5 days) in elementary computer physics for students in their freshman university year is described. The aim of the course is to remove the constraints on traditional physics courses imposed by the necessity of only dealing with problems that have simple analytic solutions. Thus it will be shown that insight into the solutions of rather complex problems can be gained by numerical experimentation and that expensive laboratory experiments may be simulated by computer experiments. A harmonic oscillator, a charge in crossed electric and magnetic fields, and a lunar space vehicle are used as examples.

INTRODUCTION

In the traditional undergraduate physics courses, where the laws of classical mechanics and elementary electricity are introduced together with the definitions of such concepts as mass, force, work, energy, charge and fields, the problems put to the students are purposefully idealized to an extent such that simple analytical solutions can be obtained. The examples used thus leave a rather academic impression, and only very few cases of practical interest can be treated. This situation is often illustrated by stating in introductory courses, that the three-body problem of classical mechanics cannot be solved analytically.

With the easy access to computers it is now possible to remove this constraint in physics courses as it is in engineering practice and we no longer need to be content with using idealized models to gain a qualitative understanding of the consequences of the basic laws of physics.

The aim of the elementary computer physics course described in the following, is to give an introduction to this new branch in physics in order to illustrate how it is possible, with easy access to a computer, to replace these traditional constraints on physics courses (that only analytically solvable problems can be used as examples) with the more modern and realistic constraints set by the available computer system.

The present, computer-based, one-week course in physics is part of a three-week noncompulsory course in physics—8 hours per day, 5 days per week—composed by choice of the students of 3 out of 5 one-week courses; the other 4 elective courses, which do not include computer calculations, have the following titles: collisions, space flight, particle optics, and the stability of the bicycle. The last is partly experimental, the others are purely theoretical. The three-week course is offered to the students at the Technical University of Denmark in their freshman year after they have completed elementary courses in mathematics, mechanics, and elementary computer science in order to deepen their understanding of the basic laws of physics. In the following, a brief description will be given of the one-week computer physics course.

To begin with we want to investigate the new tool offered by the computer and show that very accurate solutions to physical problems can be found by means of the computer using simple numerical methods. For this purpose we use an example, which has an analytical solution to compare with, viz. the simple harmonic oscillator. In the second exercise the same numerical technique is applied to an example of a physical problem closely related to some engineering problems met in practice and for which the possible solutions cannot easily be studied without the use of a computer. In the third exercise we look for numerical solutions to a problem which has no analytical solutions, and here a lunar space vehicle is used as an example with the additional inherent possibility of illustrating most aspects of classical mechanics.

In the course we use an alphanumeric screen terminal connected to an IBM 370/165 installation. The jobs, which run under a fast filehandling system, have a turn around time of up to a few minutes. Workable "raw" programs which include a line plot facility in order to be able to visualize the results are put at the disposal of the students so that it is possible to start without wasting time on programming. The programs have no input/output statements. The physical parameters of the system under study are changed directly in the program as part of the numerical experiments. The programming language used is FORTRAN IV.

HARMONIC OSCILLATOR

The harmonic oscillator is used to obtain experience with some very simple integration algorithms, and to learn the level of accuracy which can be obtained with different choices of time step and machine precision. With the position, velocity, and acceleration of the oscillator known at a given time t, we can determine the velocity and position a time step Δt later. The simple Euler method

$$v(t + \Delta t) = v(t) + a(t)\Delta t, \qquad (1a)$$

$$x(t + \Delta t) = x(t) + v(t)\Delta t, \qquad (1b)$$

where in general $a(t) = a(x(t), v(t))$, is easy to understand but has poor efficiency, i.e., the time step Δt should be rather small in order to gain accurate results. We compare the numerical results obtained by the Euler method, the midpoint rule also called the "leapfrog" algorithm.[1,2]

$$x(t + \Delta t) = x(t) + v(t + \Delta t/2)\Delta t \qquad (2a)$$

$$v(t + 3\Delta t/2) = v(t + \Delta t/2) + a(t + \Delta t)\Delta t \qquad (2b)$$

and the results obtained by the second-order Taylor method[3]

$$v(t + \Delta t) = v(t) + a(t)\Delta t + (1/2)\{[a(t) - a(t - \Delta t)]/\Delta t\}(\Delta t)^2, \qquad (3a)$$

$$x(t + \Delta t) = x(t) + v(t)\Delta t + (1/2)a(t)(\Delta t)^2, \qquad (3b)$$

with the analytical solution for the harmonic oscillator. It is obvious what we mean when we talk about the error in the position of the particle at a particular time, but what is the error of an approximate function $y_c(t)$ compared with the true function $y(t)$? A suitable measure, satisfactory for practical purposes, is the L_p-norm,[4] defined for the range $t_1 \leqq t \leqq t_2$ by

$$L_p = \left(\int_{t_1}^{t_2} |y_c(t) - y(t)|^p \, dt \right)^{1/p}, \qquad (4)$$

where p is a constant in the range $1 \leqq p \leqq \infty$.

In practical applications, the reason for preferring one value of p to another is generally a matter of convenience; we use the value which is most convenient. Most attention has been paid to the $p = 2$ and $p = \infty$ norms. A low value of L_p corresponds to a good approximation.

Before starting the harmonic oscillator exercise the choice of a criterion for the accuracy of the numerical solution is discussed with the students.

As a measure of accuracy the absolute value of the largest difference between the numerically integrated, and the exact, values of the particle positions or the sum of squares of these differences for each step divided by the number of steps in a period are usually suggested by the students. More seldom, the sum of the absolute values of the differences is suggested. These criteria correspond to the $p = \infty$, 2 and 1 L_p-norms, respectively. The first criterion is also known as the minimax and the second as the least-square criterion.

The students are asked to use the three algorithms with a number of different time step values Δt in each case, and in single precision (S) as well as in double precision (D), and to make a graphical comparison. Figure 1 shows, in logarithmic scale, the maximum error of the results obtained for the position of the particle in the first period, as obtained by one group of students. The error is measured relative to the amplitude. It is seen that the Euler method gives an error proportional to the time step Δt (slope = 1), whereas the midpoint rule and, not shown, the second-order Taylor method gives an error proportional to the square of Δt (slope = 2). With single precision and the midpoint rule a minimum is seen at about $\Delta t = 5 \times 10^{-3}$ s. At lower Δt the accumulated roundoff errors dominate, at higher Δt the errors due to finite Δt dominate.

The students usually spend the first two days with the harmonic oscillator.

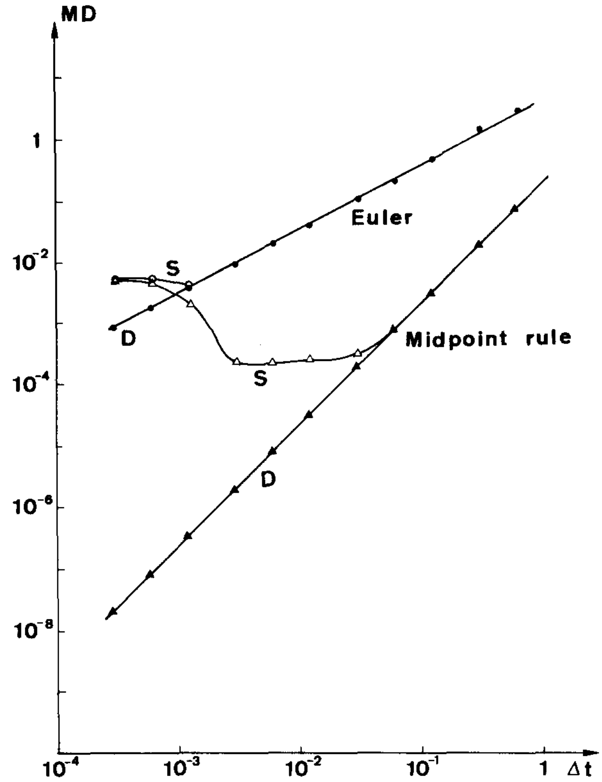

Fig. 1. The maximum error MD in the position of the particle relative to the amplitude found by numerical integrations of the harmonic oscillator equations in the first oscillation period as a function of the time step Δt used in the algorithm. The period is 6.28 s. MD is shown for the Euler and the midpoint rule algorithms in single (S) as well as in double precision (D). Results with very high relative accuracy can be obtained with these simple algorithms.

CHARGE PROPAGATION IN CROSSED FIELDS

After finishing the harmonic oscillator the students have gained some experience in simple integration methods and are ready for problems which can only be attacked numerically. We consider a moving charge in crossed magnetic and electric fields, a problem relevant for a number of important devices, e.g., the magnetron, the mass spectrometer, the getter-ion pump, and the Penning ionization gauge. It does not matter that the particular example chosen has in fact an analytical solution,[5] as this is not easy to find for the freshman students, and it is not used in this course.

We have the equation of motion

$$m(d\mathbf{v}/dt) = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}), \qquad (5)$$

where m and q are, respectively, the mass and the electric charge of the moving particle, $\mathbf{v}$ is the velocity, $\mathbf{E}$ and $\mathbf{B}$ are, respectively, the intensities of the electric field and the magnetic field. We choose for convenience $\mathbf{E}$ along the x axis, $\mathbf{E} = E\mathbf{u}_x$, and $\mathbf{B}$ along the z axis, $\mathbf{B} = B\mathbf{u}_z$, and $\mathbf{v} = (v_x, v_y, v_z)$, then

$$m(d\mathbf{v}/dt) = qE\mathbf{u}_x + qv_yB\mathbf{u}_x - qv_xB\mathbf{u}_y. \qquad (5a)$$

The Cartesian components of the velocity can thus be determined numerically from the equations

$$m(dv_x/dt) = (qE + qv_yB), \qquad (6a)$$

$$m(dv_y/dt) = -qv_xB, \qquad (6b)$$

$$m(dv_z/dt) = 0. \qquad (6c)$$

From one time step in Eq. (6a) we get a v_x which is used in Eq. (6b) and vice versa. v_z is constant so we only consider a projection in the XY plane.

We now simulate an experimental setup, in which we can adjust the magnitude of m, q, $\mathbf{E}$, and $\mathbf{B}$ and the magnitude and direction of the initial velocity $\mathbf{v}_i$. The students are asked to give a description of the path of the particle from the line plot generated in the "raw" program, and very soon they realize that the drift velocity $\mathbf{v}_D$, defined as the average velocity over several periods, is a useful parameter. An illustrative example of such a plot is shown in Fig. 2. This parameter is then studied by numerical experiments, i.e., by varying the other parameters within chosen limits, the behavior of the function $\mathbf{v}_D = \mathbf{v}_D(m,q,\mathbf{v}_i,\mathbf{E},\mathbf{B})$ is determined.

Some further information can be extracted by small

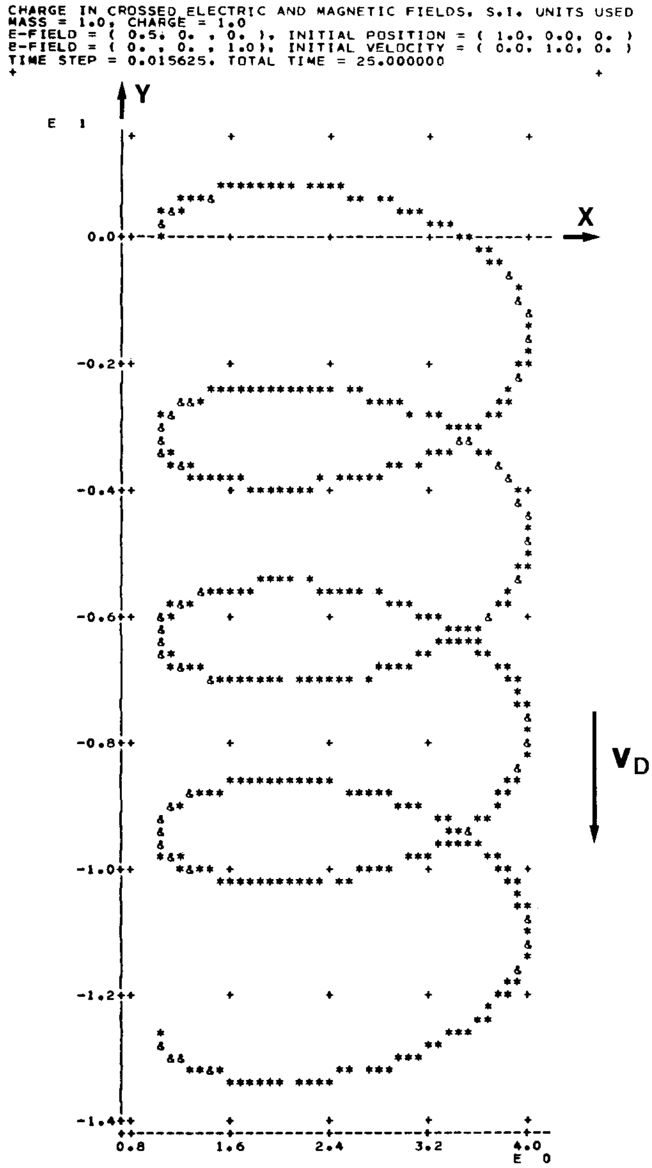

Fig. 2. Line plot of the projection of the trajectory of a charge in crossed electric and magnetic fields in the XY plane. A useful parameter is the drift velocity $\mathbf{v}_D$ defined as the average velocity of the charge over several periods. The direction of $\mathbf{v}_D$ is indicated on the figure. The electric field **E** is along the x axis, the magnetic field **B** along the z axis perpendicular to the plane of the paper. The midpoint rule is used.

changes in the computer program. One can investigate whether the accuracy is satisfactory in relation to the determination of the drift velocity either by inspecting the line plot and comparing whether the different cycles are alike, or by calculating the total energy and checking whether it is preserved within the numerical accuracy aimed at. One can make a line plot in the $v_x v_y$ plane or in a frame of reference moving with the drift velocity $\mathbf{v}_D$.

This second problem is usually finished after the third day or sometimes after three and a half days from the beginning of the course.

LUNAR MISSION

As a somewhat more advanced problem the lunar space vehicle[6] is used as an example of a problem with no analytical solution. In order to simplify the problem we assume that the space vehicle trajectory is situated in the Earth-Moon orbital plane and that the Moon's orbit is approximated by a circle. The space vehicle initially orbits around the Earth and from this parking orbit the velocity of the spacecraft is changed by a rocket burn so that it leaves the orbit tangentially. We assume that the time used for the rocket burn is negligible compared to the time of flight to the Moon. Thereafter the space vehicle, with a given initial velocity, moves according to the laws of gravitation, i.e., the vehicle trajectory is now ballistic. The integration technique used is the second-order Taylor method as described by Grauer and Tanis,[3] except that we do not keep the Moon in a fixed position in our treatment.

The students choose a frame of reference. Either they use a nonrotating coordinate system with the origin at the center of the Earth, or they use a rotating coordinate system again with the origin at the center of the Earth and the x axis pointing towards the Moon.

A valuable feature of this lunar mission problem is its large inherent flexibility, i.e., the number of questions which can be answered by means of computer calculations is only limited by the time left for this exercise. The lunar mission problem is thus the time buffer of the course. Of the many illustrative questions, which can be answered by means of the lunar mission program, we shall mention a few:

(a) How can we check the accuracy of the results? (In rotating coordinates the total energy of the lunar vehicle should be preserved, or if the mass of the Moon is assumed zero the trajectory of the space vehicle should be a perfect conic section, which with a moderate initial speed would be a closed ellipse).

(b) Find the transit time to the Moon as a function of the initial velocity.

(c) Assume that the Moon moves counterclockwise around the Earth. Is it then preferable that the space vehicle traverses the parking orbit counterclockwise in order to approach the Moon easily?

(d) Try to make an impact trajectory and determine the velocity of the space vehicle at the collision time.

(e) What happens if the space vehicle passes just before the Moon in its orbit? (This results in a nonperiodic circumlunar mission and the space vehicle returns to Earth ballistically.)

(f) What happens if the space vehicle passes just behind the Moon in its orbit? (Then we have a lunar passage to escape[7] by a gravity-assisted swing-by.)

(g) Vary the numerical value and the direction of the initial velocity to see how critical the success of the mission depends upon these parameters.

DISCUSSION

The course has been attended by altogether 40 students. The number of students each week was limited as the department has only one screen terminal. The students therefore worked in groups of 3–6 persons.

The course started with an introduction to the use of the alphanumeric screen terminal, and with a general talk about the aim and contents of the computer exercises. During the week there were several discussions among which should be mentioned the problem of checking the results. The students are warned not to trust blindly the output of the computer and they are encouraged to find checking methods, for instance, by using conservation principles if applicable, e.g., conservation of energy as in the example with a charge in crossed fields, or to use the knowledge of the trajectory as an ellipse for the space vehicle with the mass of the Moon set to zero and with moderate initial velocity.

Although we only use very simple methods for solving ordinary differential equations, the students are informed about the existence of advanced methods, which are available in many subroutine libraries, and examples are given. The students finish the computer exercises by writing a short report describing the major results. Credit for the course is only given if the report is accepted.

It seems clear from the discussions with the students and from the quality of their reports that the purpose of the course as stated in the introduction was fully attained. The students seemed to have obtained a good start in computer physics so that those particularly interested had a good basis for choosing courses which could deepen their knowledge about the subject. Although the course is very concentrated it is my experience that the progress is satisfactory, the alternation between the routine work at the terminal and the creative planning of strategy on problem solution, etc. being a reasonable combination. Most of the students were very enthusiastic and worked even more than schemed. Working at the terminal is amusing and they were tempted to spend too much time here. Thus it was often necessary to warn against spending too much time on digressions from the main problems. When operating at the terminal they should preferably have a predetermined plan. It could also be necessary to prevent the students from making too few or too many points on a table or graph, or to help them choosing parameter values. Particularly in the lunar mission problem it can be difficult to choose the initial position and velocity of the space vehicle in order to have a collision with the Moon. Here a crude line plot of the trajectory is not of much help but the distance between the space vehicle and the Moon should be calculated after each time step. Without guidance the students might thus experiment for hours without success. When appropriate parameter values are determined, however, a line plot is very illustrative of minor changes of these parameters and helps to answer the questions posed in the lunar mission section.

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[1]Computer Notes, Am. J. Phys. **39,** 1409 (1971).

[2]A. W. Luehrmann, Am. J. Phys. **42,** 361 (1974).

[3]A. D. Grauer and N. B. Tanis, Phys. Teach. **12,** 169 (1974).

[4]J. G. Hayes, *Numerical Approximation to Functions and Data* (Athlone, Belfast, 1970), p. 6.

[5]L. Spitzer, *Physics of Fully Ionized Gases* (Interscience, New York, 1965), pp. 3-5.

[6]Lunar Flight Handbook, NASA SP-34, Part 1, Vol. II (1963).

[7]V. D. Barger and M. G. Olsson, *Classical Mechanics* (McGraw-Hill, New York, 1973), pp. 131-144.